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Modeling and Simulation of Plasma-Assisted Ignition and Combustion

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AFOSR MURI "*Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion*"

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Summary of 2012-2013 Progress

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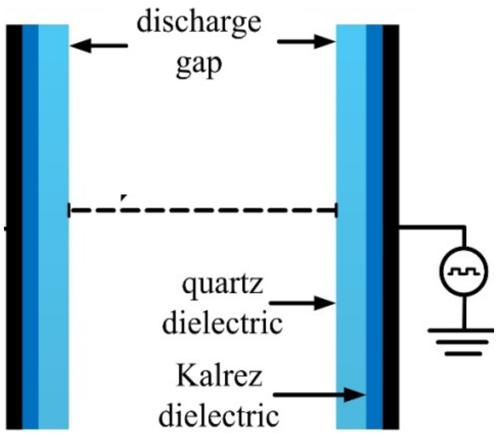
Plasma Flow Reactor



Air Plasma

- self-consistent simulations of pulsed nanosecond discharges in air.
- detailed validation with experiments and analytical model results.

•demonstration of volumetric plasma heating and radical production of critical importance in combustion applications.

Ignition of H_2-, CH_4-, and C_2H_4-Air Mixtures

•critical assessment of plasma kinetic models through comparison of OH decay rates after a burst of nanosecond pulses below ignition threshold temperatures (~500 K).

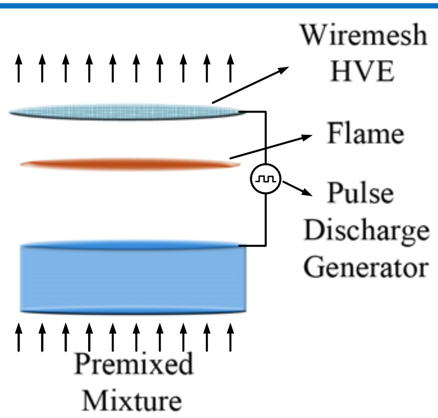
•importance of local plasma chemistry effects over heat transport in achieving "volumetric" ignition using pulse nanosecond discharges.

•detailed parametric studies on the sensitivity of nanosecond plasma ignition to pressure, eq. ratio, pulsing frequency, burst size, initial temperature, and dielectric properties.

Ignition of Heavy Fuels (n-Heptane)

- effect of nanosecond plasma on the two-stage n-heptane ignition process.

Plasma-Coupled Premixed Flames



- construction of plasma flame kinetic mechanisms, including electron impact dynamics of all major species in flame environments (both reactants and products).
- effect of species and temperature gradients in the flame zone on the spatial characteristics of the plasma (E/N, electron density etc.)
- focus on plasma radical generation in the preheat zone and the impact on overall flame characteristics.

Georgia Tech

Publications

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1. S. Nagaraja, V. Yang, I. Adamovich, "*Multi-Scale Modeling of Pulsed Nanosecond Dielectric Barrier Discharges in Plane-to-Plane Geometry*," Journal of Physics D: Applied Physics 46 (15), 2013, 155205.
2. S. Nagaraja, V. Yang, Z. Yin and I. Adamovich, "*Ignition of Hydrogen-Air Mixtures using Pulsed Nanosecond Dielectric Barrier Plasma Discharges in Plane-to-Plane Geometry*," Combustion and Flame, 2013, in press
3. S. Nagaraja, and V. Yang, "*Detailed Comparison between Nanosecond Plasma and Thermal Ignition of Hydrogen-Air Mixtures*" to be submitted to Combustion and Flame.
4. S. Nagaraja and V. Yang, "*Numerical Investigation of Nanosecond Plasma Assisted Ignition of* H_2*-,* CH_4*- and* C_2H_4*-Air Mixtures*" to be submitted to Combustion and Flame.
5. S. Nagaraja, W. Sun and V. Yang, " *Nanosecond Plasma Assisted Ignition of n-Heptane-Air Mixtures*," in preparation.

Plasma-Assisted Combustion
Modeling Framework

Model Assumptions

- Plasma fluid with drift-diffusion approximation.
- Two temperature model: electrons at T_e (defined using mean energy); ions and neutrals at gas temperature, T_{gas}
- Lookup table for electron transport and rates using two-term expansion for electron Boltzmann equation (BOLSIG).
- Solution to mean-energy equation to update electron coefficients at each time step.
- Uniform pre-ionization in the discharge volume. No photo-ionization source term.

Governing Equations

Continuity $$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

Momentum $$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + F_i^{EHD}$$

Energy $$\frac{\partial \rho \Omega}{\partial t} + \frac{\partial [(\rho \Omega + p) u_i]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + Sg$$

Species Continuity $$\frac{\partial n_k}{\partial t} + \nabla . J_k = S_k$$

Equation of State $$p = \sum_{i=1}^{N-1} \rho Y_i R_i T_{gas} + \rho Y_e R_e T_e$$

Electron Energy $$\frac{\partial n_\varepsilon}{\partial t} + \nabla . J_\varepsilon = S_\varepsilon ; n_\varepsilon = n_e \bar{\varepsilon}$$

Electric Potential $$\nabla . (\varepsilon \varepsilon_0 \nabla \varphi) = -e(n_+ - n_- - n_e)$$

Electric Field $$\vec{E} = -\nabla \varphi$$

Validity of the BOLSIG approach to calculate electron rate coefficients, among other assumptions, has been validated through comparison of species density (O and OH), temperature and input energy with experiments

Nanosecond Plasma Assisted Ignition and Combustion
Multi-Scale Modeling Framework

PLASMA DISCHARGE DYNAMICS
Plasma Chemistry
Ionization, Excitation, Dissociation, Recombination

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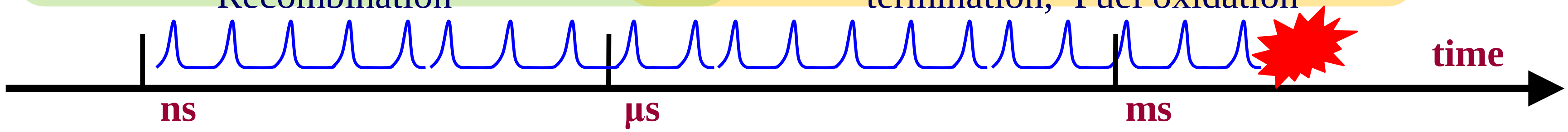
FLOW AND COMBUSTION DYNAMICS
Ignition and Combustion Chemistry
Radical initiation, Chain propagation, termination, Fuel oxidation



ns:
- ionization wave propagation
- electrical breakdown
- cathode sheath formation
- electron impact dynamics

µs:
- quenching of excited species
- ion recombination
- gas heating

ms:
- cumulative effects of multiple discharge pulses
- convective and diffusive transport
- ignition and combustion

Solution Algorithm

electric field Implicit LU decomposition → **electron energy** Implicit GMRES → **electron and gas transport coefficients** → **plasma species and flow conservation equations** → (back to) **electric field**

Strategies for Computational Efficiency

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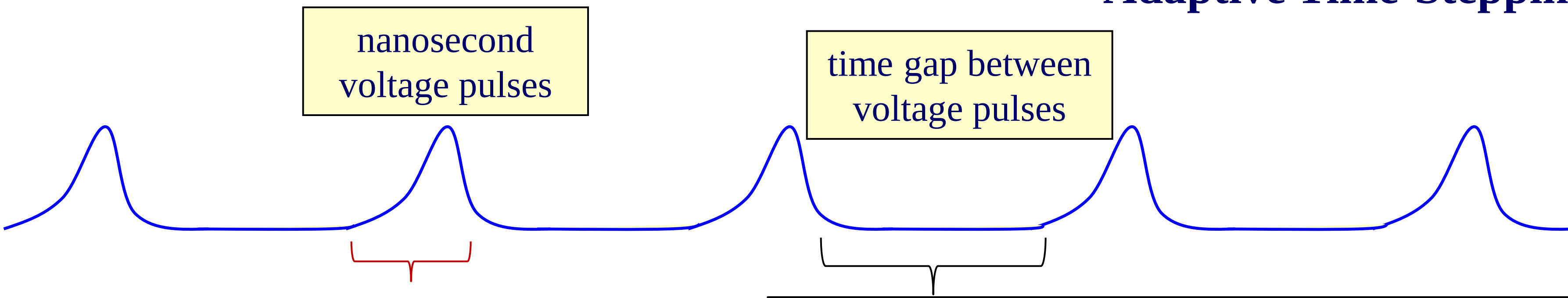
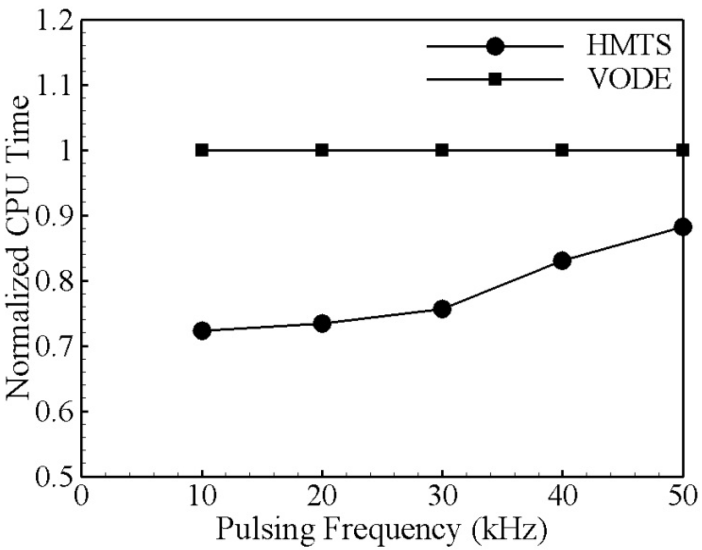
Adaptive Time-Stepping



- **Δt varies between 10^{-13} -10^{-12} s**
- **Semi-implicit treatment of the Poisson equation to circumvent the stiffness arising from tight coupling between electric field and electron density.**

- **Δt fixed at 10^{-9} s .**
- **Electron energy equation and Poisson equation are not solved since electric field effects become negligible and the space charge density rapidly decay as the applied voltage ends.**



Multi Time-Scale Treatment of Chemical Source Term

- **speedup by 40% is seen by using the multi time-scale treatment of chemical source terms, but not orders of magnitude speedup observed in combustion simulations without plasma discharge.**
- **at high pulsing frequencies, the savings with using HMTS reduce because more time spent in simulating electric field transients during breakdown in each voltage pulse.**

*** Gou et al., Combustion and Flame 157 (2010) 1111–1121**

Strategies for Computational Efficiency

plasma combustion chemistry optimization

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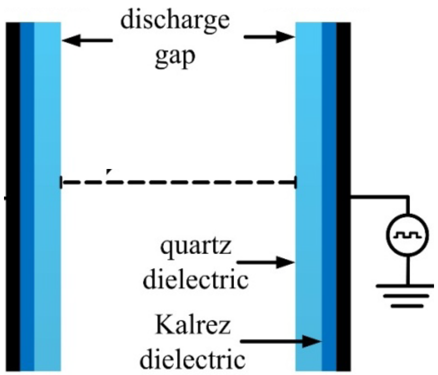
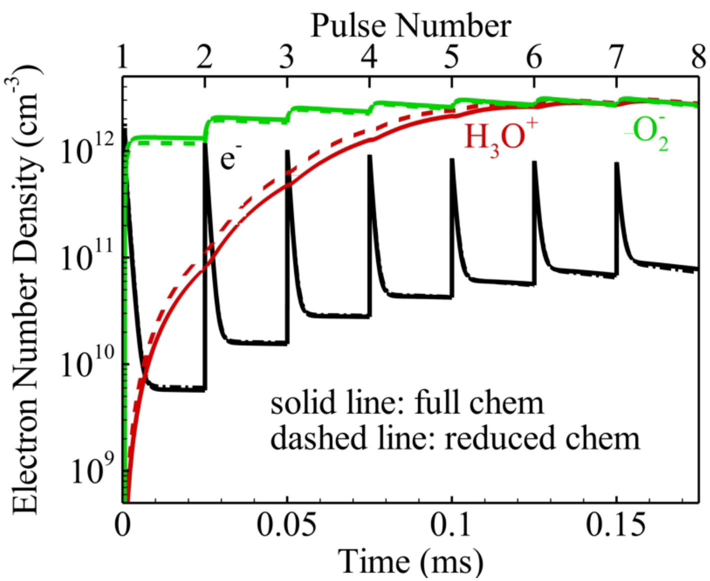
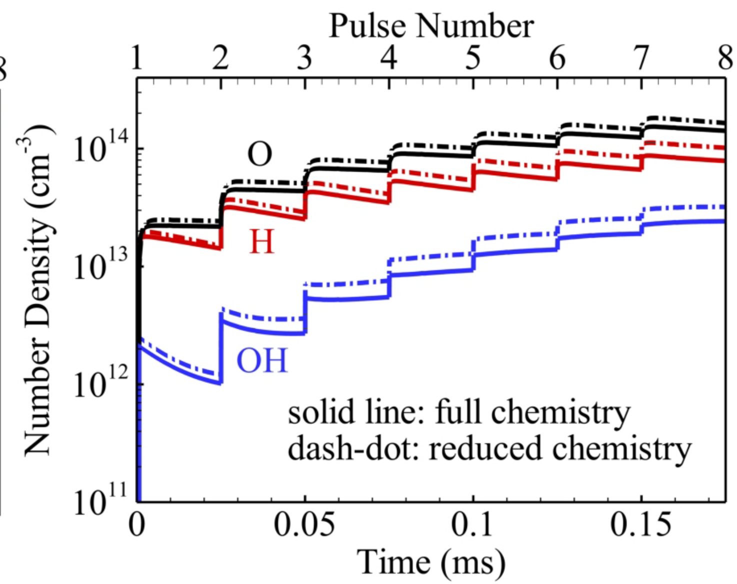


H_2-air
$\phi = 1$
94 torr
473 K
8 pulse burst

charged species densities at center of discharge gap



O, H and OH densities at center of discharge gap



full chem: 35 species, 287 reactions   optimized chem: 19 species 111 reactions

- simulated a burst of 8 nanosec pulses with detailed mechanism.
- removed species with peak mole-fraction less than 10^{-8}
- **ensured that E/N, electron and radical species densities and temperature (in both space and time, all within 10%) are accurately predicted by the reduced mechanism.**
- provides a speed-up of ~ 4 times with H_2-air plasma ignition.
- expect greater savings with large C_xH_y mechanisms and 2D/3D simulations.

OSU Plasma Flow Reactor

40 - 160 torr, 300 - 500 K, 1 - 100 kHz

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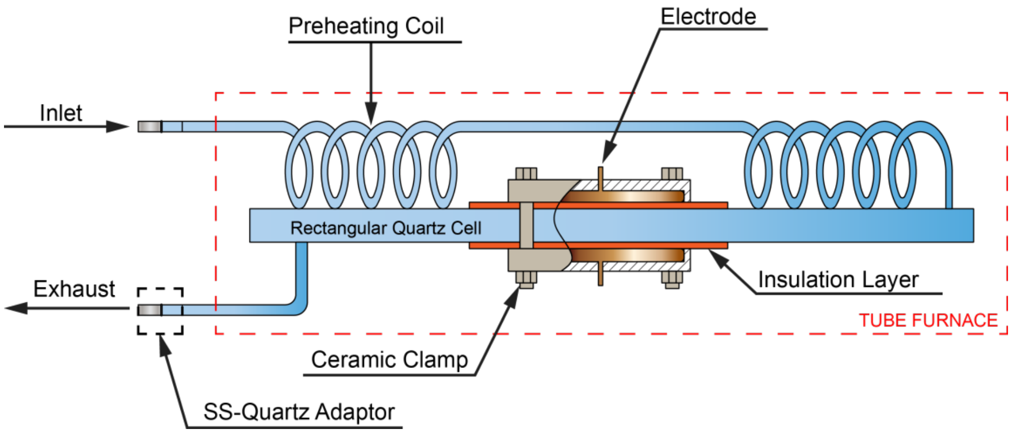


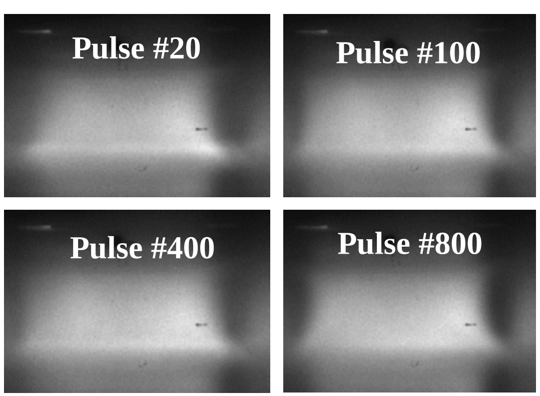
measurements

- **time resolved O density** using TALIF (uncertainty +/- 30%)
- **time resolved NO density** using LIF (uncertainty +/- 30%)
- **time resolved OH density** using LIF (uncertainty +/- 20%)
- **time resolved temperature** using rotational CARS and/or LIF thermometry
- **ignition delay time** from OH* emission rise
- **ICCD imaging** of discharge structure and flame kernel evolution.

ICCD images of discharge structure

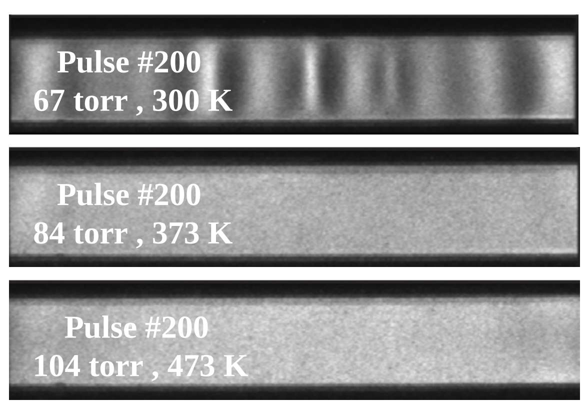
Front View (2 cm × 1 cm)

Air : 373 K, 60 torr, 40 kHz

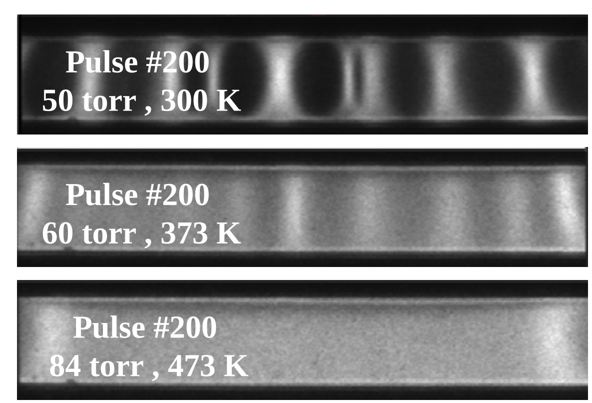


Side View (6 cm × 1 cm)

H_2 - Air : 40 kHz

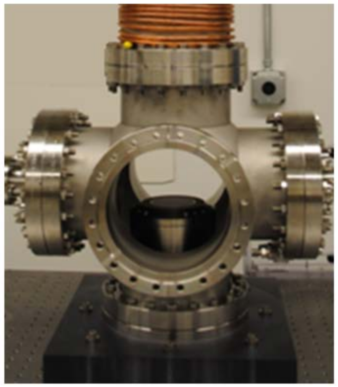


C_2H_4 - Air : 40 kHz

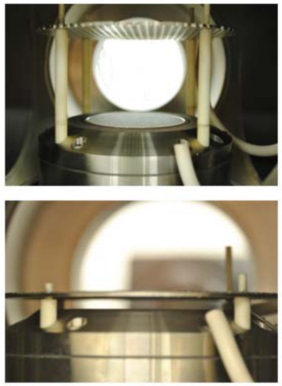


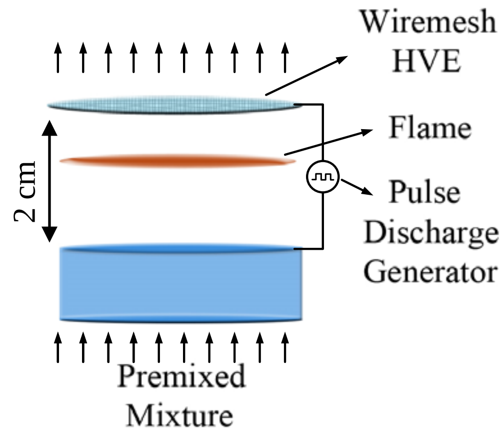
OSU Plasma-Coupled Premixed Flat Flame

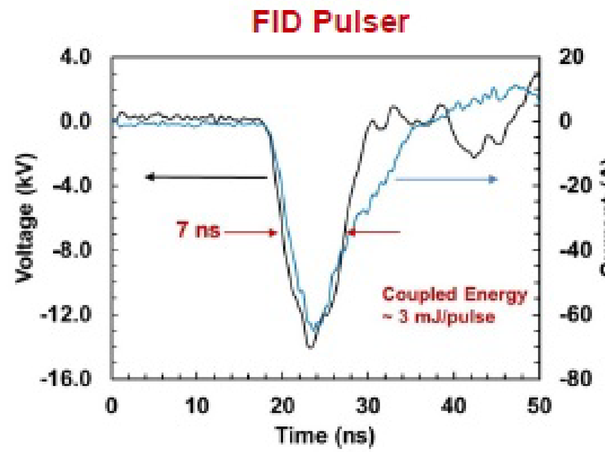
Facility



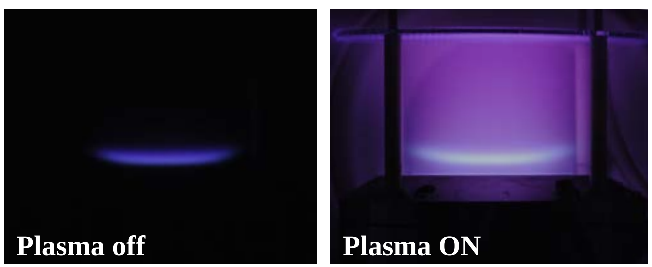
Burner Configurations



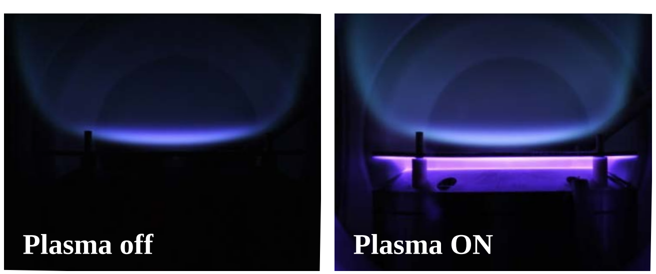




"direct coupled" configuration



"plasma upstream" configuration



- low pressure 1D flame (20 - 30 torr)
- $H_2/O_2/N_2$, $CH_4/O_2/N_2$ and $C_2H_4/O_2/N_2$ premixed flames
- FID pulser: 14 kV peak voltage, 7 ns FWHM, ~3 mJ/pulse

Measurements

- **spatially resolved OH density** using LIF
- **spatially resolved temperature** using five-line OH thermometry.

Nanosecond Pulsed Dielectric Plasma Simulations in N_2/Air

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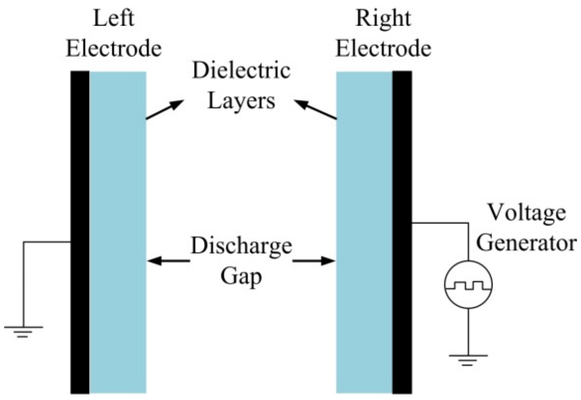
Objectives

- Self-consistent simulations of pulsed nanosecond discharges in air with detailed kinetics.
- Validation with experiments and analytical model results.
- Direct insight into plasma heating and radical production of critical importance in combustion applications.

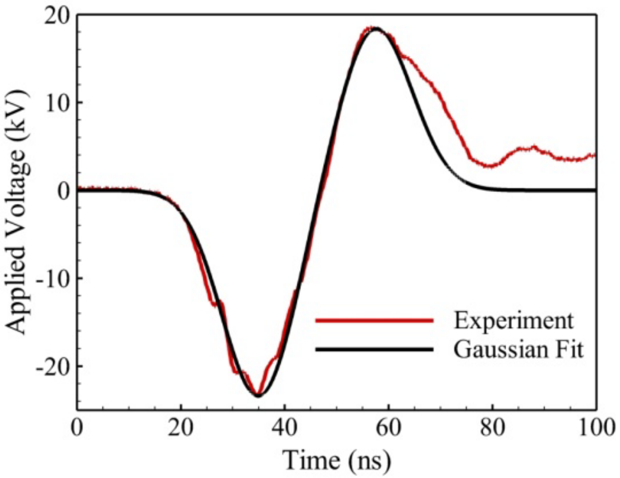
Model Geometry



Operating Conditions:

Initial Pressure: 60 torr
Initial Temperature: 300 K
Pulsing Frequency: 40 kHz
Gap width: 1 cm
Initial Electron Density: 10^7 cm^{-3}
Dielectric thickness: 1.75 mm
Dielectric Constant: 4.3
Pulse Duration: 100 ns, FWHM: 12 ns
Peak Voltage: -22.5 kV and +17.5 kV

Applied Waveform



S. Nagaraja, V. Yang, I. Adamovich, "*Multi-Scale Modeling of Pulsed Nanosecond Dielectric Barrier Discharges in Plane-to-Plane Geometry*," Journal of Physics D: Applied Physics 46 (15), 2013, 155205.

Experimental Validation (Air Discharge)

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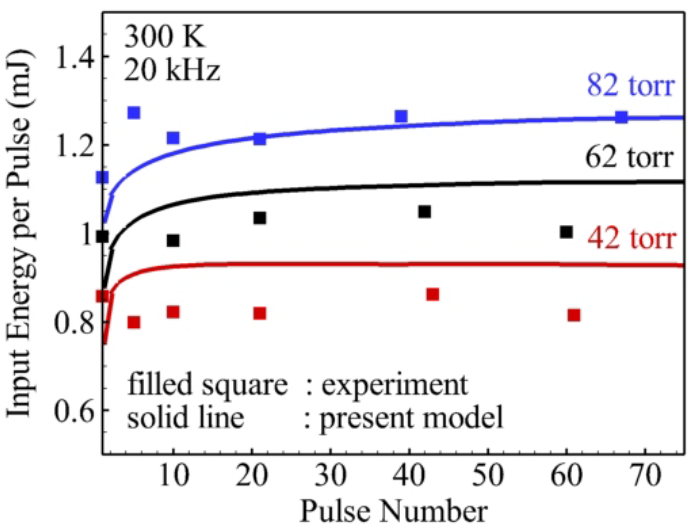
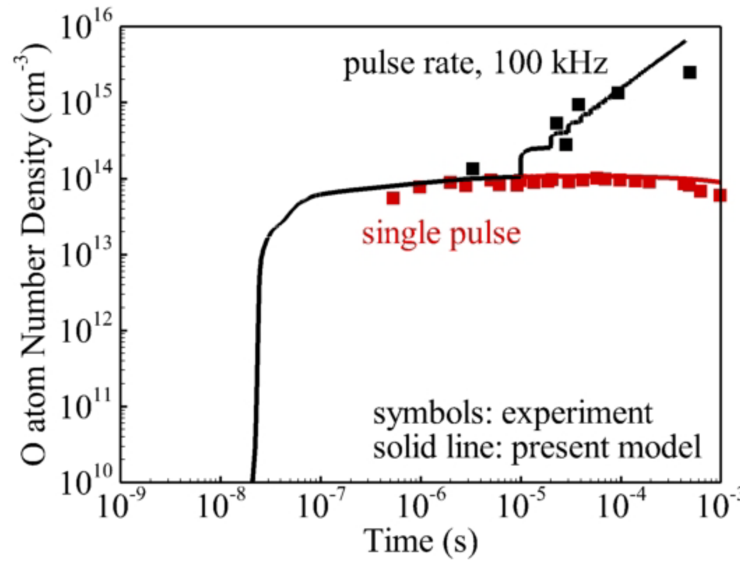
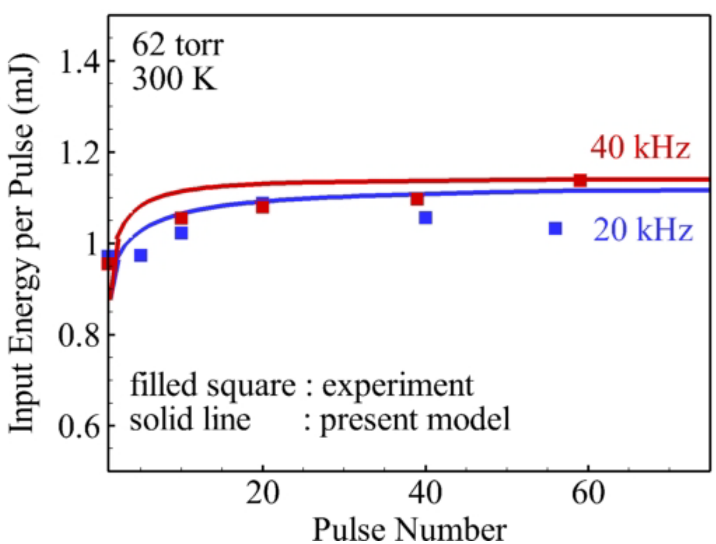
Coupled Pulse Energy



O density at center of discharge volume





- coupled energy, temperature and O atom density predicted by the 1D model are within 20, 5 and 10% of experimental data, respectively.
- coupled energy remains fairly constant with pulse number, increasing linearly with pressure, and nearly independent of pulsing rates.
- O atom production via electron impact dissociation and quenching of excited N_2 by O_2 is captured accurately along with subsequent decay via formation of O_3 over ms timescales.

Detailed Physics over ns-ms Timescales
air discharge (60 torr, 300 K, 40 kHz, 100 pulses)

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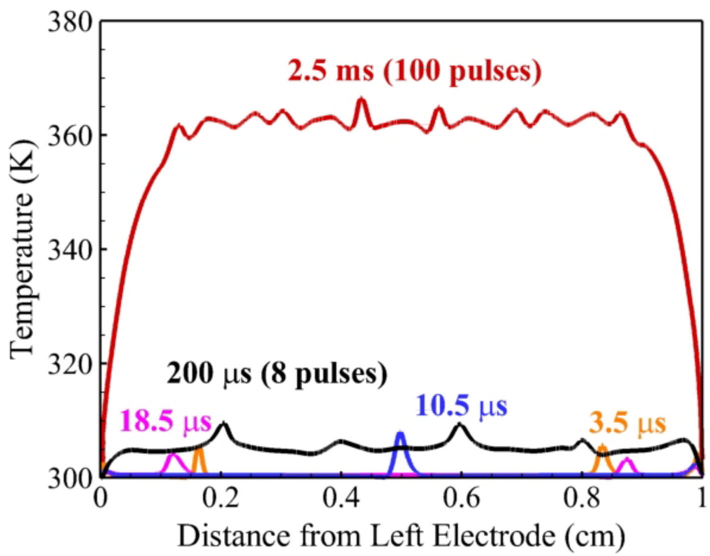
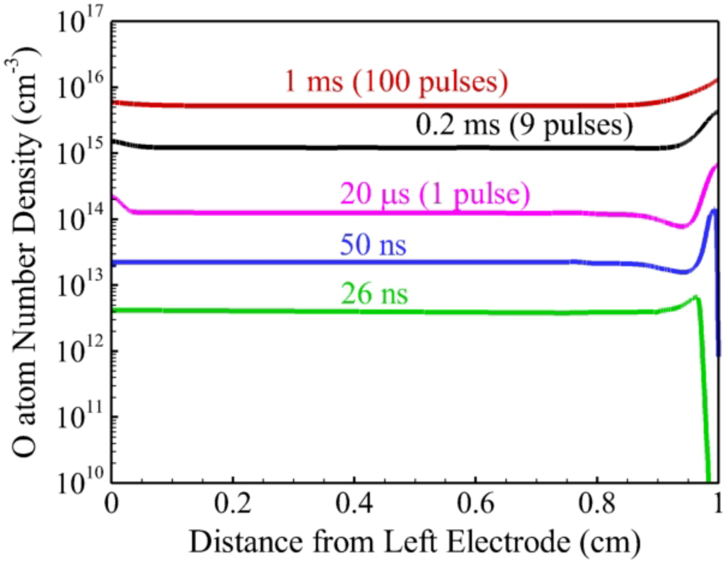
temperature evolution for 100 nanosecond pulses



spatial distribution of O atom density for 100 nanosecond pulses



- plasma heating effect is about 0.5 - 1K/pulse in air and nearly independent of pulsing frequency (as a function of pulse number).
- rapid gas heating produces weak acoustic waves which propagate into the gas volume from both ends. The strength of these waves becomes weak as overall temperature rises from heat release from quenching of excited species.
- a fairly uniform temperature profile develops in the plasma volume after several discharge pulses, owing to slow but steady (~0.5 K/pulse) heat release primarily from relaxation of excited species.
- repetitive pulsing results in efficient production of atomic oxygen through electron impact dissociation during discharge pulses, and quenching of excited nitrogen species by oxygen.
- **volumetric radical generation and heating by pulsed discharges are of great significance for ignition and flame stabilization purposes.**

Nanosecond Pulsed Dielectric Plasma in H_2-Air Mixtures

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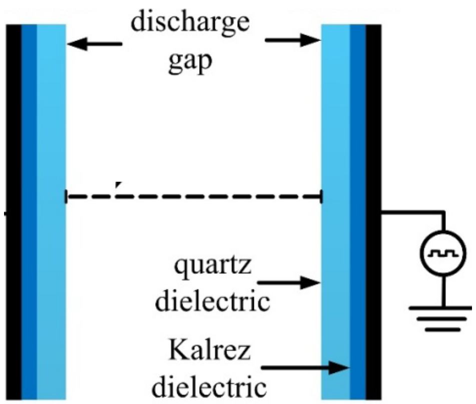
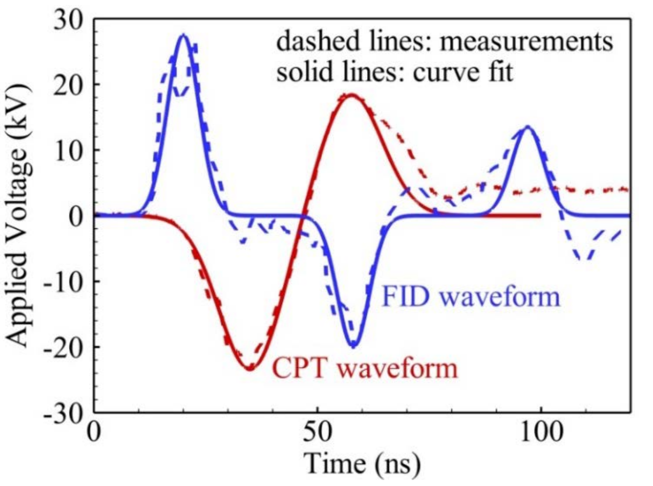
model geometry



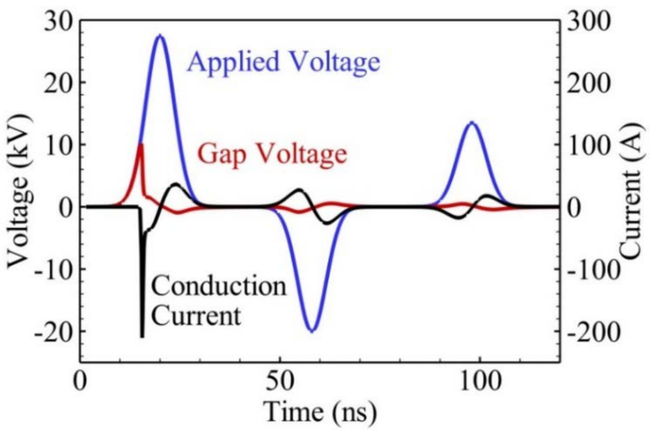
operating conditions

Pressure: 40 - 160 torr
Temperature: 373 - 600 K
Pulsing Frequency: 10 - 40 kHz
Gap width: 1 cm
Initial Electron Density: 10^7 cm^{-3}
Dielectric thickness (Quartz): 1.75 mm
Dielectric thickness (Kalrez): 1.58 mm
Dielectric Constant (Quartz): 4.3
Dielectric Constant (Kalrez): 4 - 9

applied waveforms



voltage and current



Objectives

- **comparison of OH density with measurements after a burst of 50 pulses.**
- **assess the accuracy of kinetics model at low temperature, pre-ignition conditions**
- **detailed investigations of NS plasma ignition physics and chemistry.**
- **sensitivity of ignition process to key system parameters and material properties.**

S. Nagaraja, V. Yang, Z. Yin and I. Adamovich, "*Ignition of Hydrogen-Air Mixtures using Pulsed Nanosecond Dielectric Barrier Plasma Discharges in Plane-to-Plane Geometry*," Combustion and Flame (accepted).

H_2-Air Plasma Combustion Kinetics

$H_2/O_2/N_2$ Combustion

Popov (2008) + Konnov (2008) for NOX chemistry

chain initiation

$H_2 + O_2 \rightarrow HO_2 + H$

$H_2 + O_2 \rightarrow OH + OH$

$H_2 + M \rightarrow H + H + M$

chain branching

$HO_2 + H \rightarrow OH + OH$

$HO_2 + H \rightarrow H_2O + O$

$HO_2 + O \rightarrow O_2 + OH$

$H_2 + OH \rightarrow H_2O + H$

$O + H_2O \rightarrow OH + OH$

$H + O_2 \rightarrow O + OH$

$O + OH \rightarrow H + O_2$

$O + H_2 \rightarrow H + OH$

$H + OH \rightarrow O + H_2$

three body reactions

$H + O_2 + M \rightarrow HO_2 + M$

$O + H + M \rightarrow OH + M$

$O + OH + M \rightarrow H_2O + M$

$H + H + M \rightarrow H_2 + M$

$O + O + M \rightarrow O_2 + M$

NOX reactions

$N_2 + O \rightarrow N + NO$

$N + O_2 \rightarrow NO + O$

$NO + HO_2 \rightarrow NO_2 + OH$

+

$H_2/N_2/O_2$ Plasma

dissociation/excitation

$N_2 + e \rightarrow N(^4S) + N(^2D) + e$

$N_2 + e \rightarrow N_2(A^3, B^3, C^3, a^1) + e$

$O_2 + e \rightarrow O + O + e$

$H_2 + e \rightarrow H + H + e$

ionic reactions

$N_2 + e \rightarrow N_2^+ + e + e$

$N_2^+ + H_2 \rightarrow HN_2^+ + H$

$HN_2^+ + H_2O \rightarrow H_3O^+ + N_2$

$H_3O^+ + e \rightarrow H_2O + H$

quenching of excited species

$N_2(A^3) + O_2 \rightarrow N_2 + O + O$

$N_2(B^3) + H_2 \rightarrow N_2(A^3) + H_2$

$N_2(a^1) + H_2 \rightarrow N_2 + H + H$

$N(^2D) + O_2 \rightarrow O(^1D) + NO$

$N_2(A^3) + O \rightarrow N + NO$

$O(^1D) + H_2 \rightarrow OH + H$

nonequilibrium plasma chemistry → **low temperature radical chemistry** → **high temperature combustion chemistry**

- **low temperature (500-1000 K) uncertainties in many key chain branching reactions.**
- **detailed chemistry mechanism has 35 species and 287 reactions.**
- **reduced chemistry mechanism has 19 species and 111 reactions.**

E/N and Electron Density Evolution
P_i = 80 torr, T_i = 500 K, f = 60 kHz, Φ = 1.0, FID Pulser

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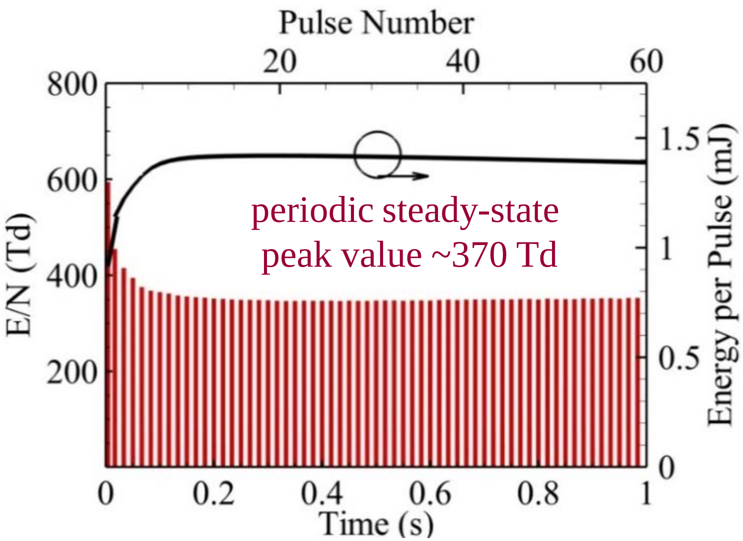
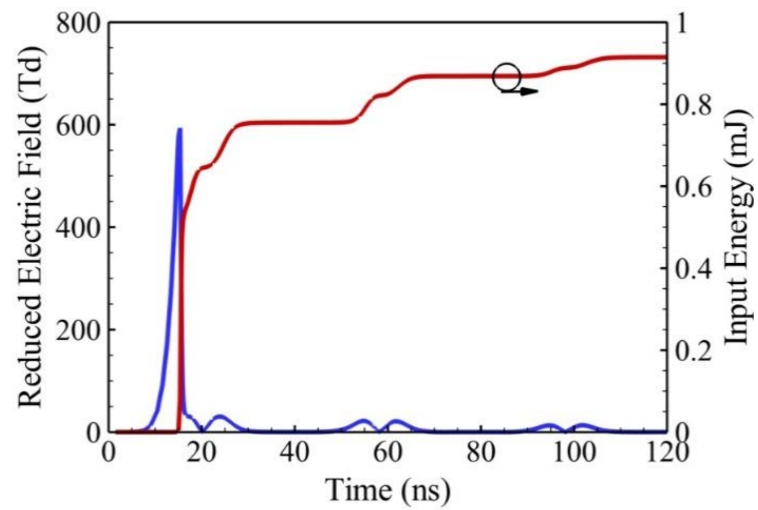
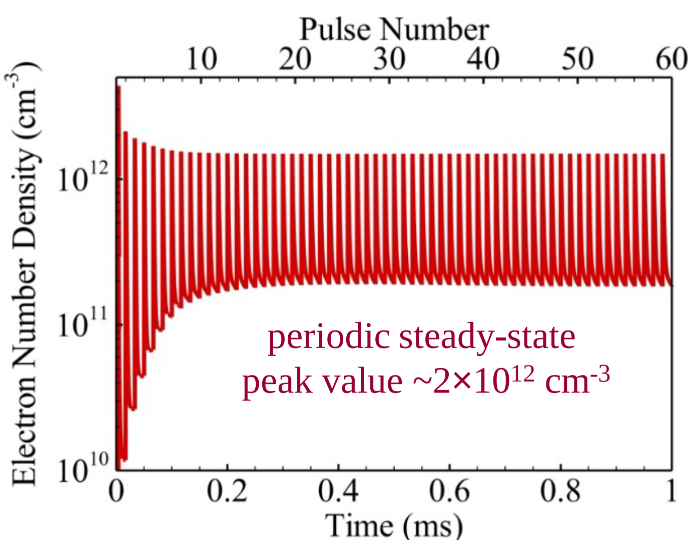
E/N at center (60 pulses)



E/N at center and input energy (first pulse)



electron density at center (60 pulses)



- **breakdown voltage at these conditions occurs at ~10 kV**
- **sharp spike in current is seen at breakdown before it drops rapidly from the plasma shielding.**
- **plasma excited species production happens only during a short duration of ~5 ns when E/N is high.**
- **E/N and electron density reach a periodic steady state after ~8 pulses.**
- **nanosecond discharge efficiently generates radicals and excited species during each pulse because of high peak E/N.**

Decay Rates of O, H and OH after a 50 pulse burst in H_2-air

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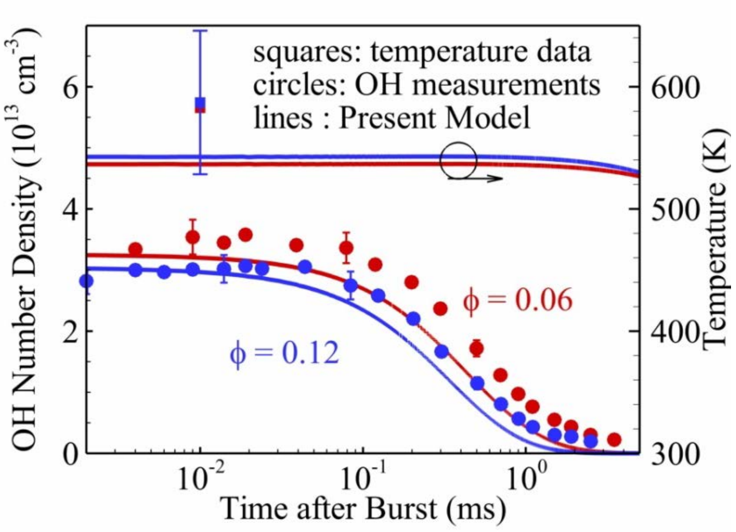
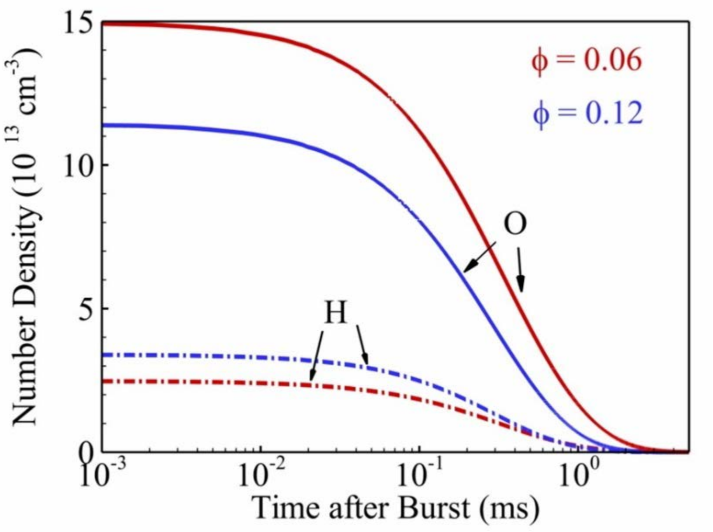
P_i = 100 torr, T_i = 500 K, f = 10 kHz, FID pulser

OH density at center of discharge gap



O and H density at center of discharge gap



key low temperature pathways for consumption of O and recirculation of H and OH

$$H + O_2 + M \rightarrow HO_2 + M \qquad O + HO_2 \rightarrow OH + O_2$$

$$H + HO_2 \rightarrow OH + OH \qquad OH + O \rightarrow H + O_2$$

- model predictions for OH are within 10% of measurements in H_2-air mixtures, including both peak value and decay rates.
- O production is highly sensitive to changes in eq. ratio, increasing by ~50% when ϕ is decreased from 0.12 to 0.06.
- H and OH are relatively insensitive, changing by ~10 % when eq. ratio is doubled.

How is ignition achieved with nanosecond plasma?

P_i = 80 torr, T_i = 500 K, f = 60 kHz, Φ = 1.0, FID pulser, 115 pulses ~ 2 ms

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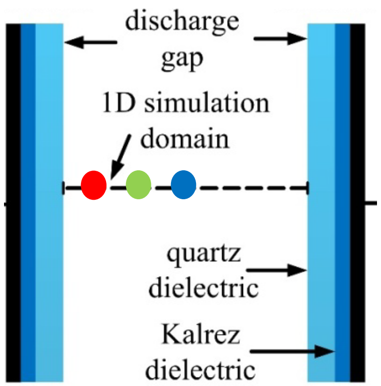
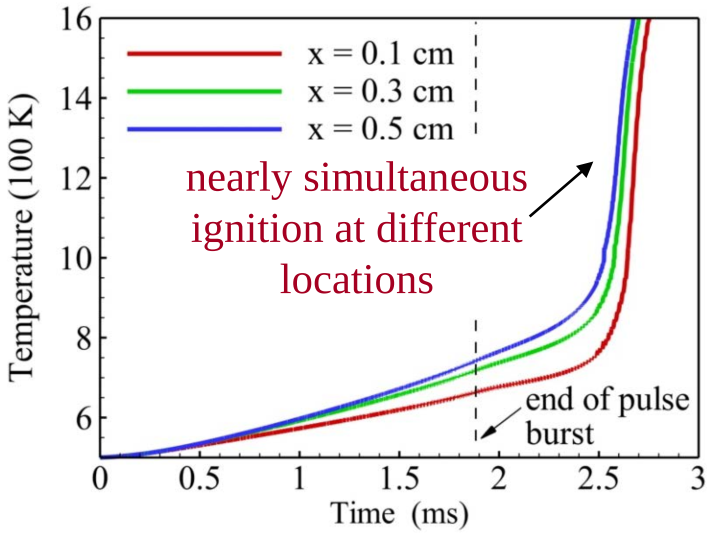
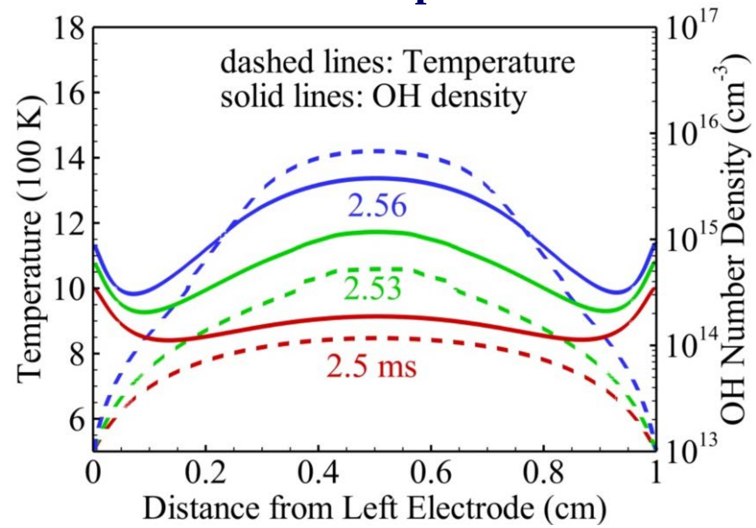


temperature evolution vs time



spatial evolution of OH and temperature



nanosecond plasma pulses → creates a pool of O, H, and OH radicals; (linear heating regime) increases temperature to a threshold value of ~700 K → (nonlinear heating regime) partial fuel oxidation is triggered → ignition and complete fuel oxidation

- heat transport plays a minor role. local plasma chemistry effects are critical in producing “volumetric” ignition
- secondary peaks in OH density near the boundaries is generated from HO_2 which has accumulated due to low temperatures

Spatial Evolution of Radicals during H_2-Air Ignition

P_i = 80 torr, T_i = 500 K, f = 60 kHz, Φ = 1.0, FID pulser, 115 pulses ~ 2 ms

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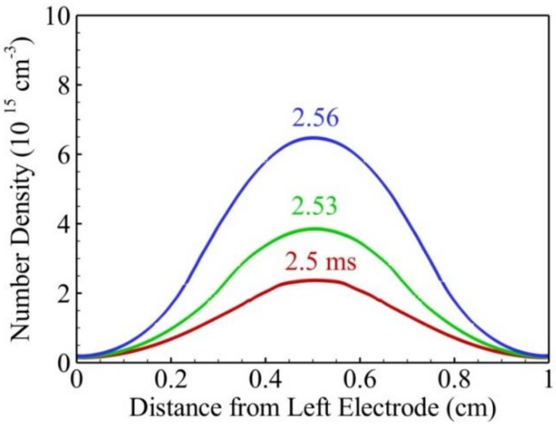
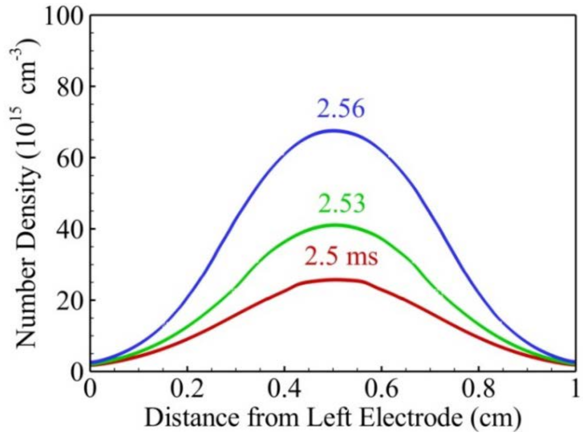
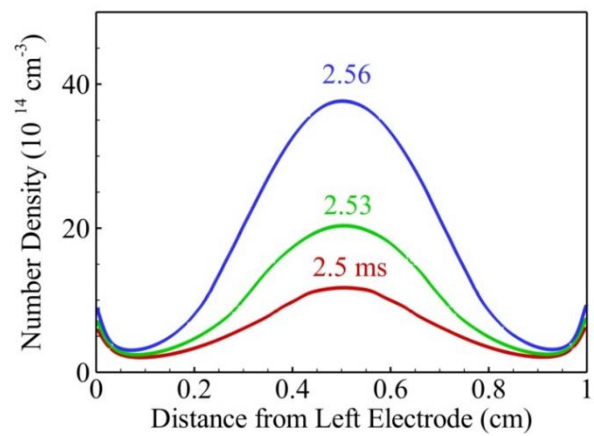
O



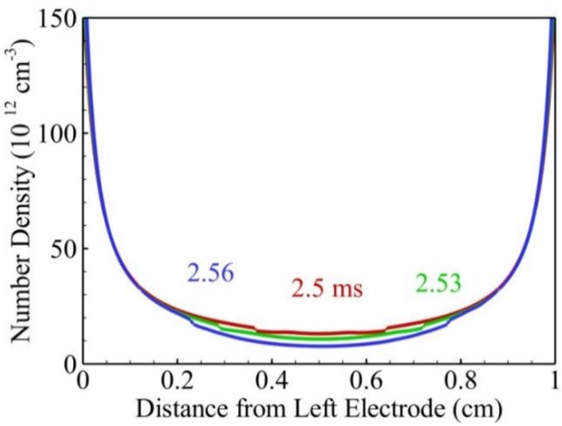
H



OH



HO_2



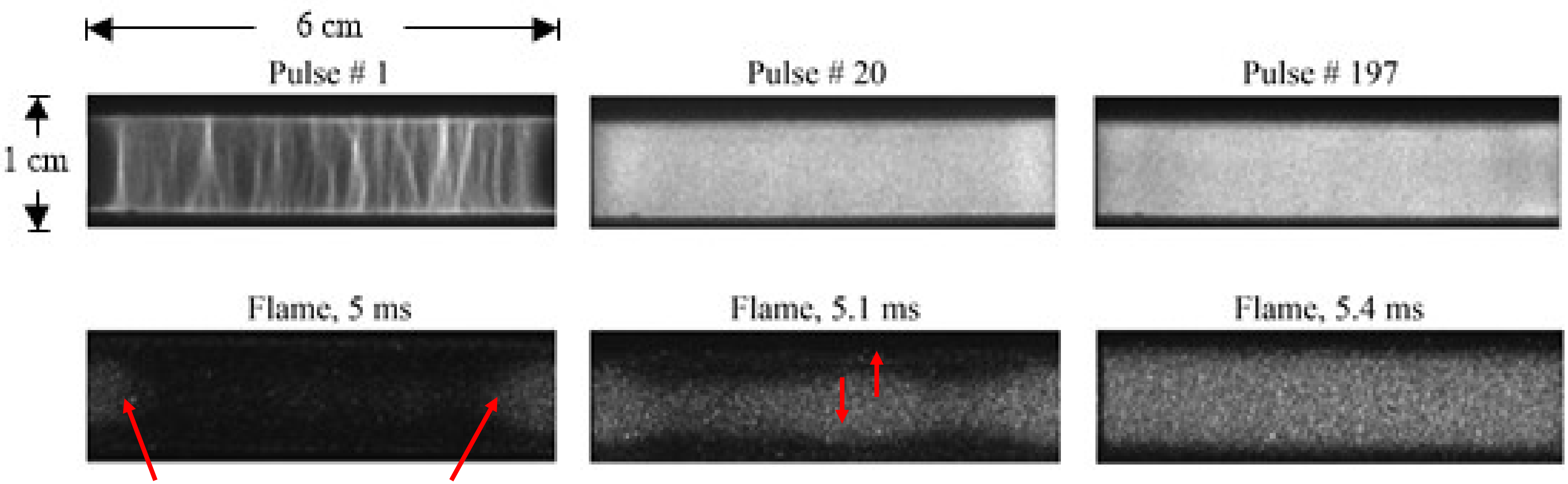
- a small increase in temperature near ignition significantly increases the chain branching reaction rates.
- radical concentration profiles are much steeper than the temperature distribution, with well pronounced maxima near the centerline.
- both O and H densities increase by ~3 times within 0.4 ms near ignition, with OH density increasing by 4 times.
- low temperatures at the boundaries because of heat losses aid the accumulation of HO_2 which generates OH. The secondary peaks in OH profiles near the boundaries result from this pathway.

H_2-air pulsed nanosecond plasma ignition

what can we infer from emission images?

OSU Experiment

P_i = 104 torr, T_i = 473 K, f = 40 kHz, Φ = 1.0, CPT pulser



ignition first observed near edges, due to higher electric fields

within 0.1 ms, ignition observed all along the centerline.

the entire volume ignited within 0.4 ms of first detected flame emission.

- the present 1D model simulates a particular cross-section.
- although the 1D model cannot capture edge effects, it is able to explain the spreading of the ignition kernel from the centerline towards the boundaries.
- predictions are in line with observations that local plasma chemistry dominate over heat transport effects

Nanosecond Plasma Ignition vs Thermal Ignition
is there any difference?

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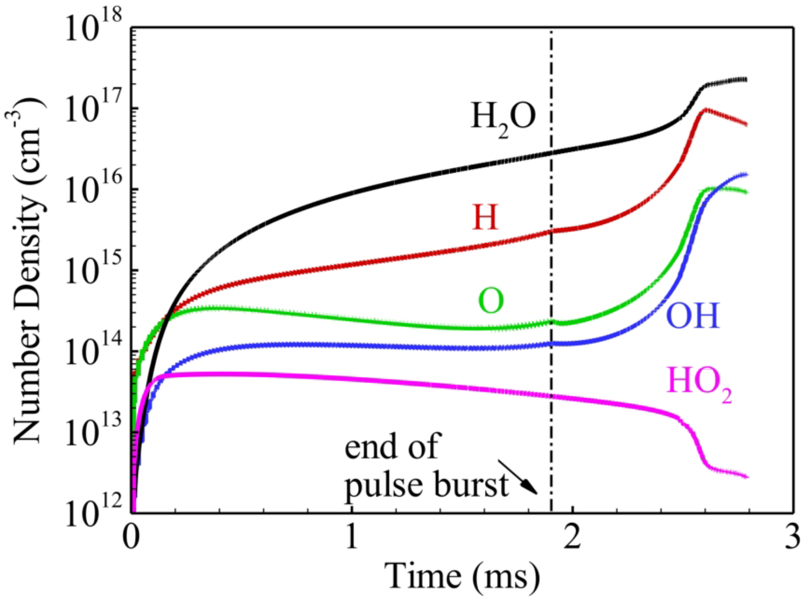
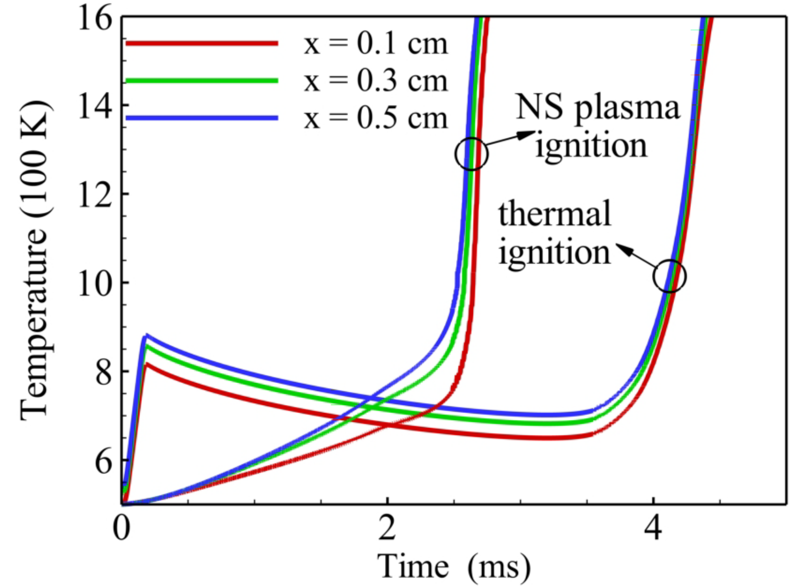
P_i = 80 torr
T_i = 500 K
f = 60 kHz
Φ = 1.0
FID pulser
115 pulses

species evolution at center for NS ignition



ignition delay times with nanosecond plasma and a volume heat source



steps in the nanosecond plasma ignition process

$N_2 + e \rightarrow N_2(A^3, B^3, C^3)$
$H_2 + e \rightarrow H + H$
$O_2 + e \rightarrow O + O$

➡

$N_2(A^3) + O_2 \rightarrow O + O(D)$
$N_2(B^3,C^3) + H_2 \rightarrow H + H$

➡

$O + OH \rightarrow H + O_2$
$O + HO_2 \rightarrow OH + O_2$
$H + HO_2 \rightarrow OH + OH$

➡

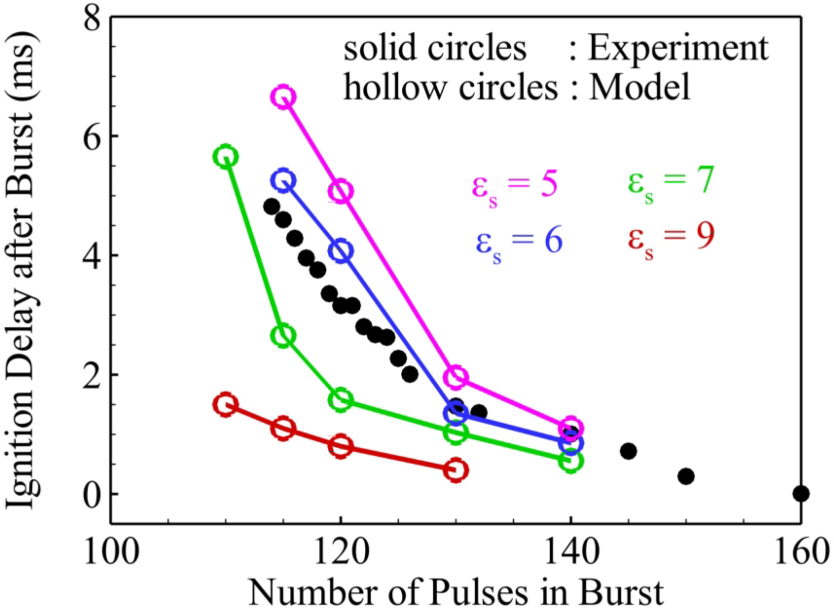
$H_2 + OH \rightarrow H_2O + H$

- the high activation energy chain initiation reactions are replaced by electron impact reactions with NS plasma.
- for the same input energy, thermal ignition delay is ~ 60% higher.
- plasma generated radicals trigger heat release from fuel oxidation at ~700 K, as opposed to auto-ignition temperature of ~960 K under same conditions.

Effect of Burst Size and Dielectric constant on Ignition

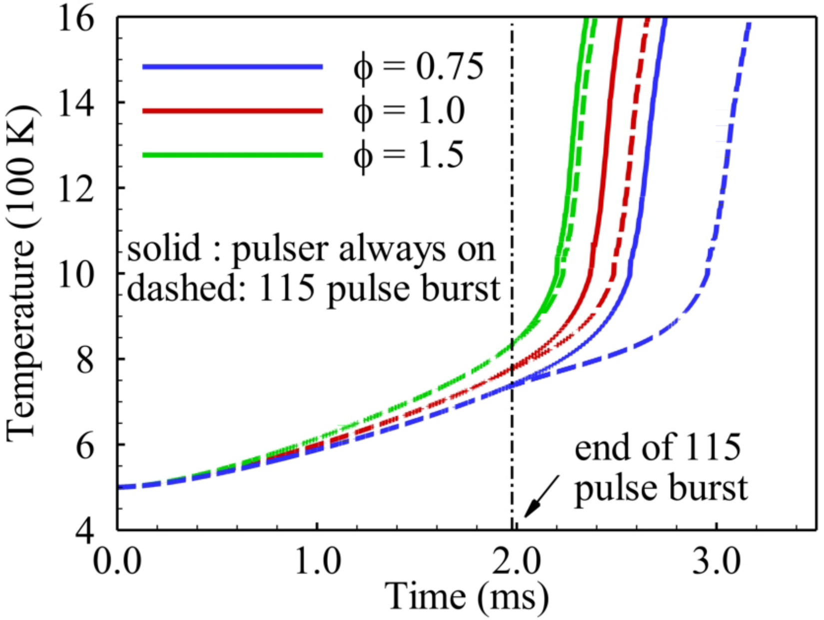
ignition delay vs # pulses in burst

P_i = 80 torr, T_i = 473 K
f = 40 kHz, Φ = 1.0, CPT pulser



ignition delay sensitivity to eq. ratio

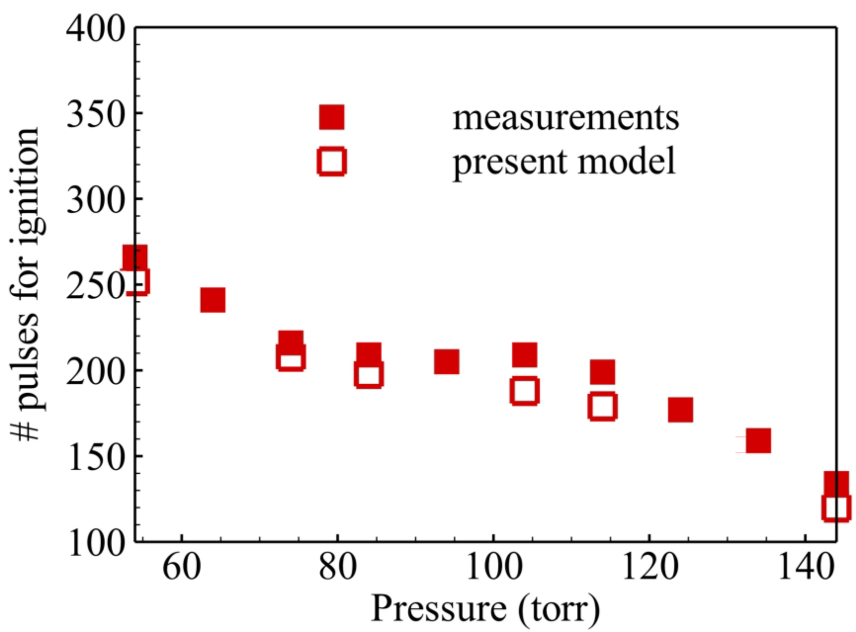
P_i = 80 torr, T_i = 500 K
f = 60 kHz, FID pulser



- there is a minimum # of pulses in burst, below which no ignition is observed.
- ignition characteristics are highly sensitive to dielectric properties.
- uncertainty in the dielectric constant values should be considered during the validation process.
- ignition delay reduction with increase in burst size is especially pronounced for lean mixtures.

Effect of Pressure and Pulsing Rates on H_2-Air Ignition

T_i = 473 K, f = 40 kHz, ϕ = 1.0, CPT pulser



- ignition delay reduction with increase in pressure is well reproduced by the model.
- increase in pressure results in nearly linear rise in input energy per pulse because of its dependence on number density. Faster addition of energy results in more rapid ignition at higher pressures.
- the nonlinear trend of # pulses required for ignition as a function of pulsing frequency is not reproduced by the model.
- the model predicts that input energy per pulse is nearly independent of pulsing frequency, which may not be true.
- lowering of input energy, because of residual electron density effects, with rise in pulsing rates may explain the observed nonlinear trend.

OH Density Decay after 50 Pulse Burst in CH_4-, and C_2H_4-Air Mixtures

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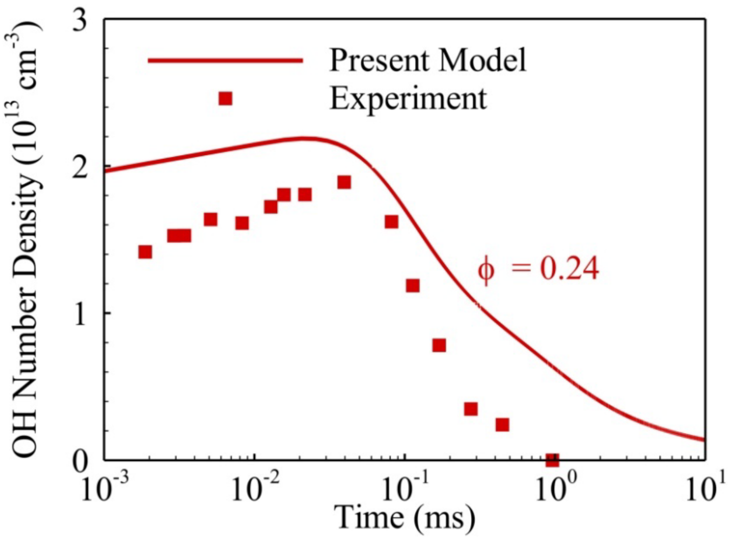
P_i = 100 torr, T_i = 500 K, f = 10 kHz, FID pulser

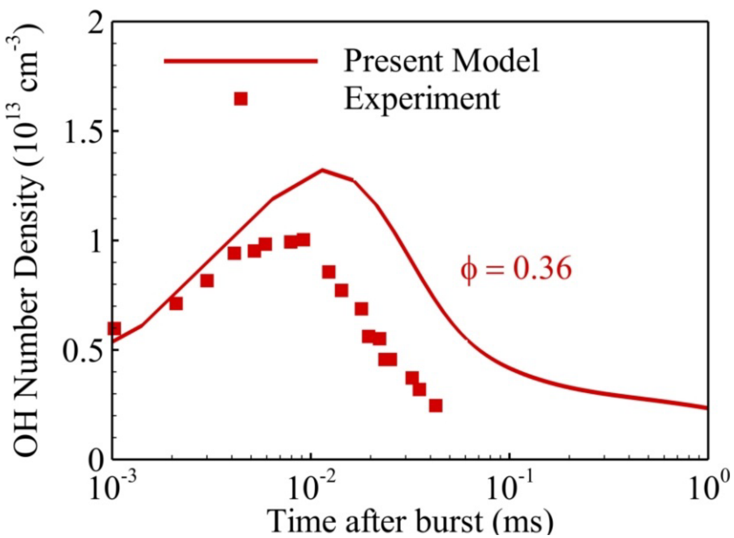
CH_4-air



CH_4-air
(64 species)
GRI Mech 3.0
$CH_4/N_2/O_2$ plasma
NOX reactions

C_2H_4-air
(70 species)
USC Mech
$C_2H_4/N_2/O_2$ plasma
NOX reactions

C_2H_4-air



- GRI Mech 3.0 has been validated extensively in 1000-2500 K and 25 torr to 10 atm range.
- USC Mech has been validated in 900-2500 K and 16 torr to 10 atm range.
- model consistently over-predicts OH density by ~50% in CH_4-air mixtures.
- growth rate is correctly predicted in C_2H_4-air mixtures, but the decay rate in slower than measurements.
- low temperature uncertainty in chain reactions may be the primary reason for deviations

Ongoing Work

- different CH_4- and C_2H_4-air combustion chemistry integrated with plasma kinetics are being tested to assess their relative performance on predicting low temperature radical production/decay.

Nanosecond Plasma Ignition of nHeptane-Air
(in collaboration with Wenting Sun)

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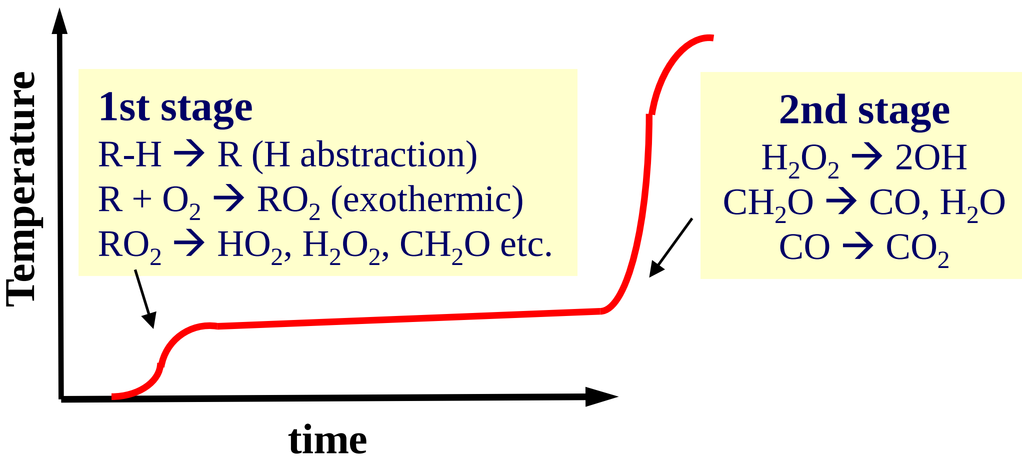

Objective

- understand the effect of NS plasma on n-heptane-air ignition chemistry through self-consistent simulations.
- investigate the effect of radical addition to the "low temperature" and "high temperature" steps of the 2-stage ignition process.

nC_7H_{16}-air plasma combustion kinetics (154 species)

$C_7H_{16}/N_2/O_2$ combustion (LLNL reduced mech + NOX reactions)

$$n-C_7H_{16}+OH \rightarrow 2-C_7H_{15}+H_2O$$
$$C_7H_{14}OOH \leftrightarrow C_7H_{14}O+OH$$
$$C_2H_3+O_2 \rightarrow CH_2CHO+O$$
$$CH_2O+OH \leftrightarrow HCO+H_2O$$
$$H+O_2 \leftrightarrow O+OH$$
$$H_2O_2+M \rightarrow OH+OH+M$$

+

$C_7H_{16}/N_2/O_2$ plasma reactions*

$$e+N_2 \rightarrow N_2(A^3,B^3,C^3,a^1)+e$$
$$e+N_2 \rightarrow N+N(^2D)+e$$
$$e+O_2 \rightarrow O+O(D)+e$$
$$e+C_7H_{16} \rightarrow C_7H_{15}+H+e$$
$$e+C_7H_{16} \rightarrow C_6H_{13}+CH_3+e$$
$$e+C_7H_{16} \rightarrow C_5H_{11}+C_2H_5+e$$
$$N_2(A^3)+O_2 \rightarrow N_2+O+O$$
$$N_2(A^3)+C_7H_{16} \rightarrow N_2+C_7H_{15}+H$$
$$N_2(A^3)+C_7H_{16} \rightarrow N_2+C_7H_{14}+H_2$$
$$N_2(A^3)+C_7H_{16} \rightarrow N_2+C_6H_{13}+CH_3$$
$$O(^1D)+C_7H_{16} \rightarrow C_7H_{15}+OH$$

* C_7H_{16} (electron impact and with excited species) reaction rates estimated from C_3H_8 based plasma reactions.

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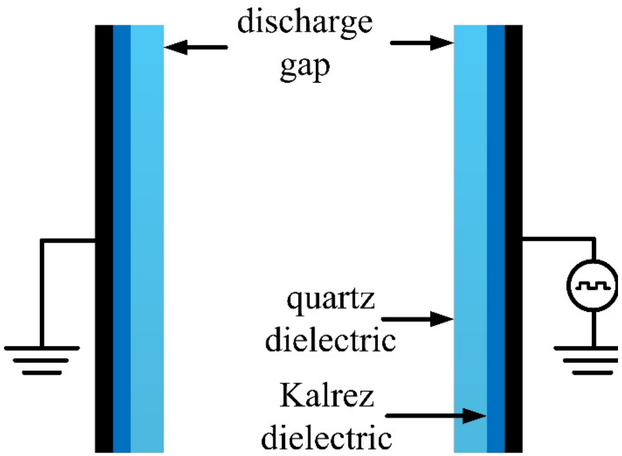
Nanosecond Plasma Ignition of nHeptane-Air

Effect of NS Pulses on 1st Stage Delay Time

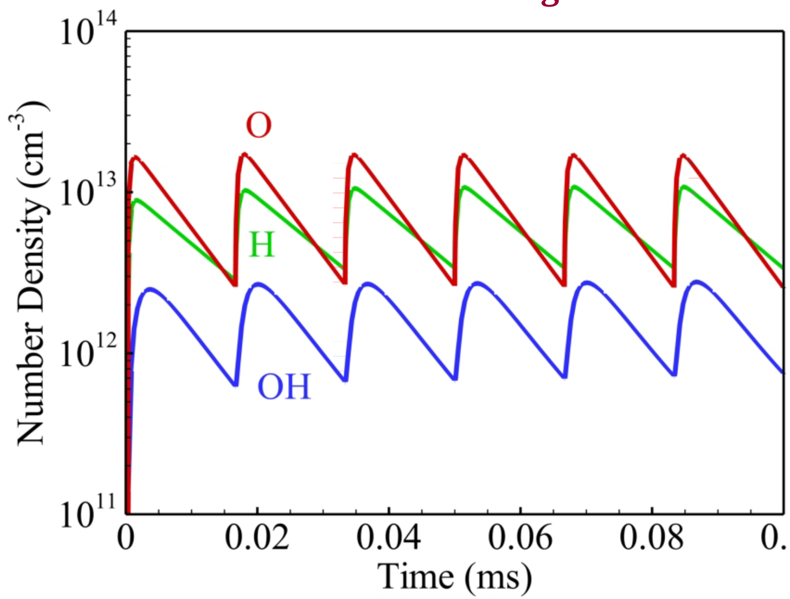
model geometry



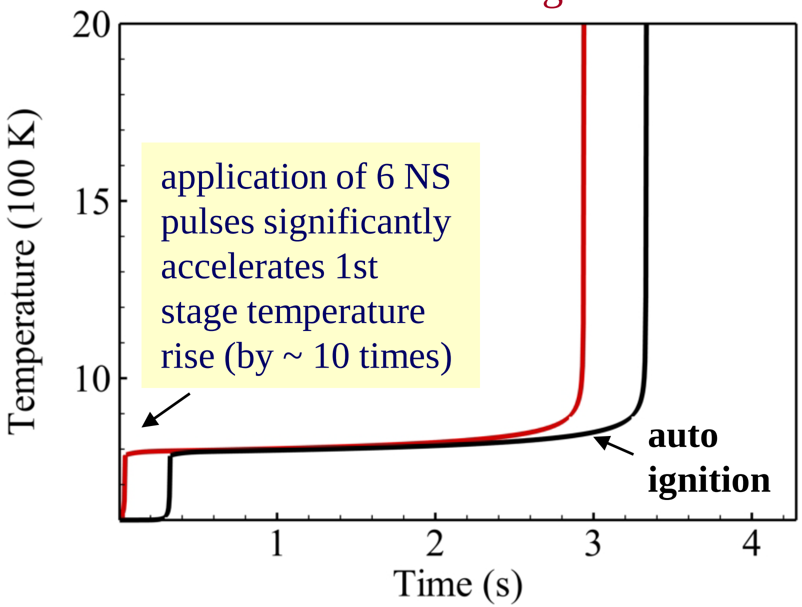
operating conditions

P_i = 160 torr
T_i = 600 K
f = 60 kHz
Φ = 1.0
8 kV Gaussian pulses
10 ns duration

O, H and OH density evolution at center of discharge volume



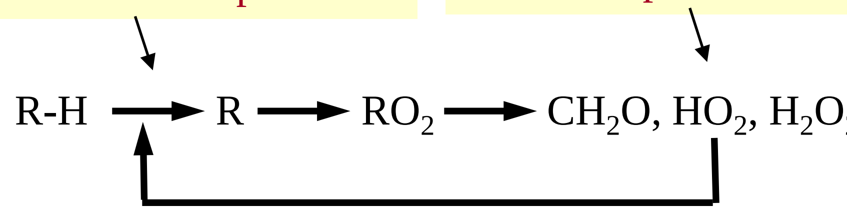
temperature evolution at center of discharge volume



"self-acceleration" of low temperature chemistry

addition of small amount of radicals accelerates the H abstraction step

RO_2 produces more radicals which accelerate the whole process further.



Nanosecond Plasma Ignition of nHeptane-Air

Effect of NS Pulses on Overall Ignition Delay Time

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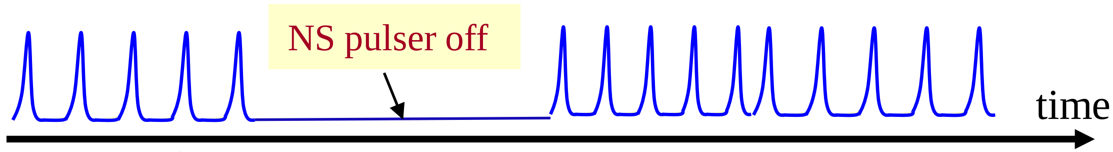
operating conditions

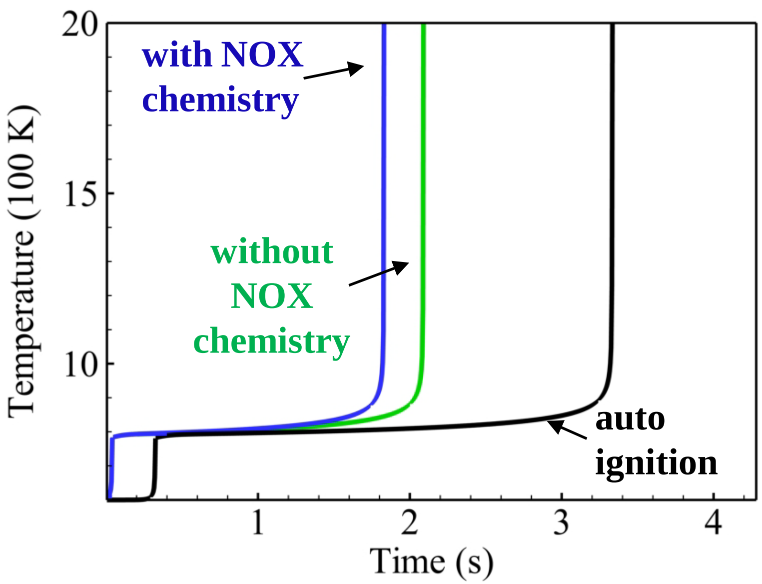
P_i = 160 torr
T_i = 600 K
f = 60 kHz
Φ = 1.0
8 kV Gaussian pulses
10 ns duration

"staggered" application of NS pulses



only a few NS pulses sufficient to rapidly trigger 1st stage temperature rise

25 NS pulses are applied after the 1st stage to reduce the overall ignition delay



- the "staggered" application of NS pulses result in ~ 40% reduction in ignition delay time
- it is evident that the 2nd stage is less sensitive to radical addition by NS pulses than the 1st stage.
- heating provided by the NS pulses after the 1st stage accelerate the decomposition of H_2O_2 and reduce ignition delay.

$$H_2O_2 + M \rightarrow OH + M$$

- inclusion of NOX catalytic reactions change the predictions by ~5% because of following new OH generation pathways.

$$NO + HO_2 \rightarrow NO_2 + OH$$

$$NO + CH_3O_2 \rightarrow NO_2 + CH_2O + OH$$

Nanosecond plasma coupled premixed flame

CH_4-air

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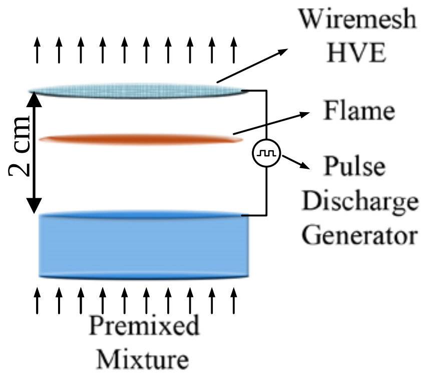
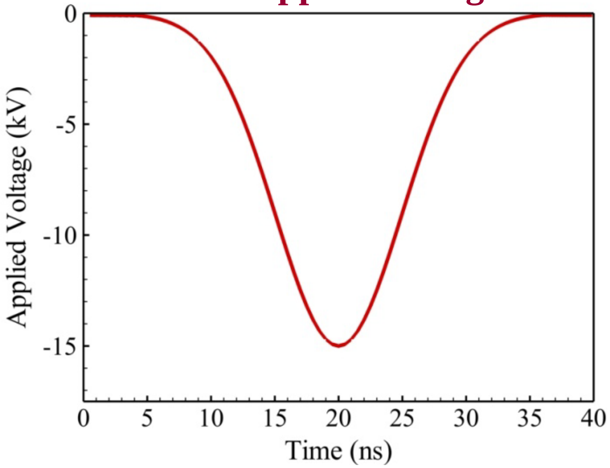
physical setup



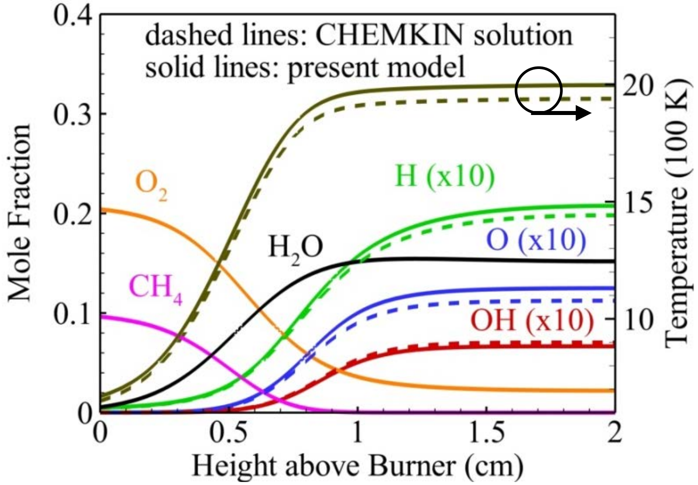
operating conditions

Pressure: 25 torr
Inlet Temperature: 650 K
Eq. ratio: 1.07
Gap width: 4.0 cm
initial Electron Density: 10^7 cm^{-3}
-15 kV peak voltage
7 ns FWHM
Mdot : 0.00377 kg/m^2-s

applied voltage



validation of flame model with CHEMKIN solution



CH_4-air plasma flame kinetics (75 species)

GRI Mech 3.0 + $CH_4/N_2/O_2/CO/CO_2$ plasma + NOX chemistry

- electron impact processes of both reactant (CH_4, O_2, N_2) and product species (H_2O, CO, CO_2) considered.

$$N_2 + e \rightarrow N_2(A^3, B^3, C^3, a^1) + e$$
$$O_2 + e \rightarrow O + O + e$$
$$CO + e \rightarrow CO^* + e$$
$$H_2O + e \rightarrow O^- + H_2$$

- what are most important plasma pathways pertaining to H_2O, CO, CO_2 ?
- is plasma species production in preheat zone more important than downstream?

Plasma Coupled Premixed CH_4-Air Flame

P_i = 25 torr, T_i = 650 K, Φ = 1.07

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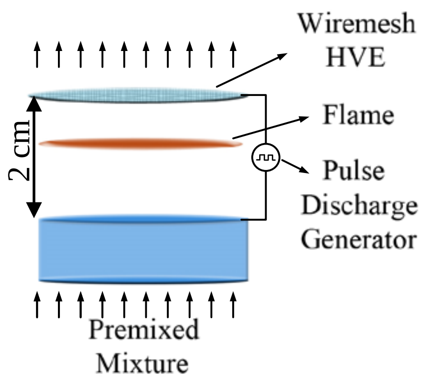
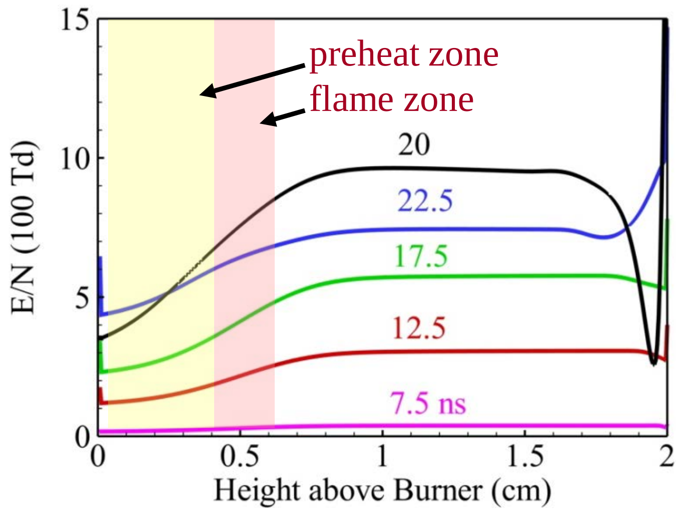
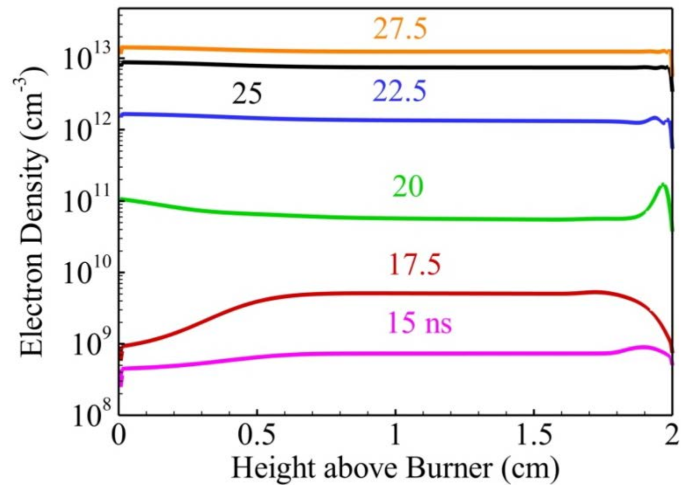
physical setup



reduced electric field vs height



electron density vs height



high E/N (100 - 600 Td) and high electron densities (~1e13 cm^{-3}) allow for efficient radical generation by NS pulses in preheat zone, where they may provide significant benefit.

note that radicals (O, H, OH etc) concentration in the flame zone is already of the order 10,000 ppm, so plasma cannot make much impact

- high E/N downstream of the flame can be attributed to high temperatures and low number density.
- E/N in the preheat zone reaches ~ 600 Td at 22.5 ns. Plasma radical generation in this zone may have a significant impact on flame characteristics.
- sharp peak in the E/N profile at 20 ns at the right boundary indicates the cathode sheath region.
- electron density distribution is fairly uniform in the entire domain reaching peak value of 2×10^{13} cm^{-3} at 27.5 ns.
- total input energy during the pulse was 2.7 mJ

Plasma Coupled Premixed CH_4 - Air Flame

P_i = 25 torr, T_i = 650 K, Φ = 1.07

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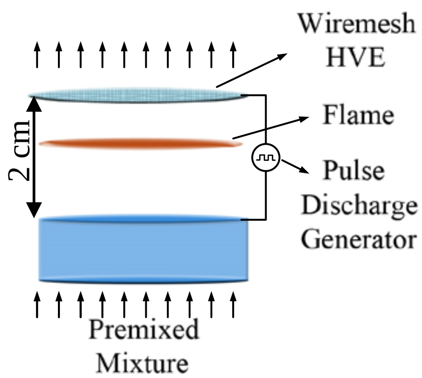
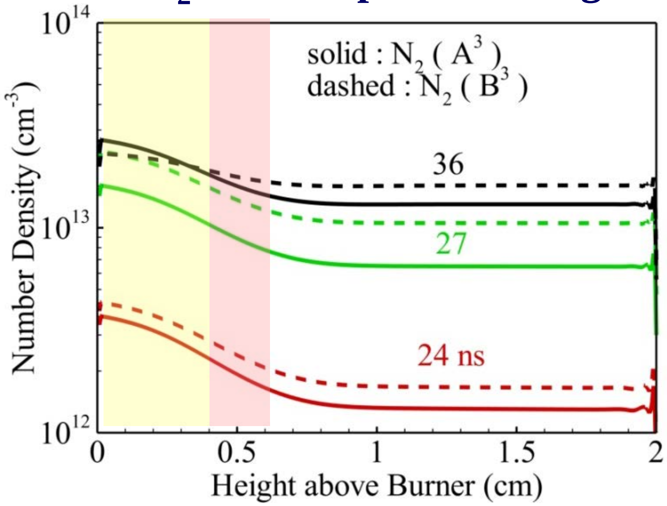
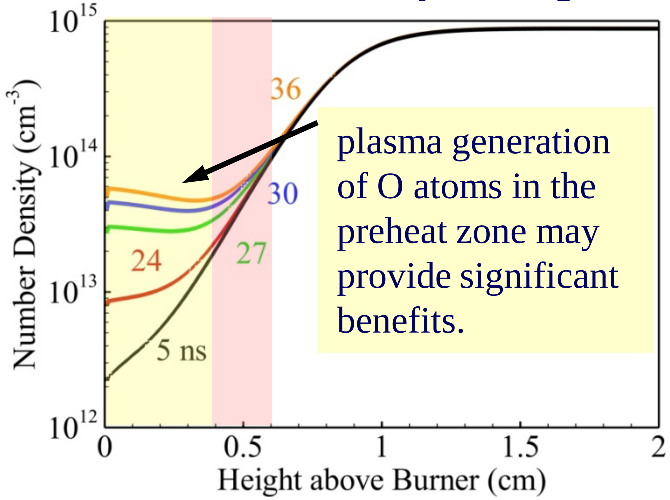
physical setup



N_2 excited species vs height



O atom density vs height



- the production rates of $N_2(A_3)$ and $N_2(B_3)$ in the preheat zone is about 2 times higher than downstream because of higher N_2 number density.
- electron impact dissociation of O_2 in the preheat zone results in ~30 times increase in O atom density within 30 ns
- the excited species are quenched rapidly after the pulse resulting in further production of O and other radicals

ongoing work

- we are performing longer timescale simulations to understand the effect of repetitive application of discharge pulses on flame dynamics.
- the effect of NS discharges on H_2-air, CH_4-air and C_2H_4-air premixed flames are being investigated.
- close collaboration with OSU group is pursued for obtaining greater insight through experiments and high fidelity modeling

Where we go from here?

High fidelity 1D numerical tools for construction and validation of robust plasma combustion kinetic models

- detailed studies of the plasma coupled premixed flame system for a variety of fuels.
- development of the counterflow plasma flame simulation framework.
- close collaboration with other MURI team members for model validation and critical assessment of the plasma combustion kinetic models

2D/3D simulations of nonequilibrium plasma in complex flow environments

- High fidelity simulations of single filament discharge in 2D with detailed chemistry.
- Large Eddy Simulation (LES) of H_2 jet in supersonic O_2 crossflow in the presence of a nanosecond plasma source.
- theoretical framework to understand plasma-flow interactions.